

Spatial differentiation of chemical removal rates from air in life cycle impact assessment

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Abstract

Purpose Spatial differentiation is a topic of increasing interest within life cycle assessment (LCA). For chemical-related impacts, in this paper, we evaluate the relative influence of substance properties and of environmental characteristics on the variability in the environmental fate of chemicals using an advanced, spatially resolved model. The goal of this study is to explore spatial distribution and spatial variability of organic chemicals, assessing the variability of the removal rate from air with a multimedia spatially explicit model Multimedia Assessment of Pollutant Pathways in the Environment (MAPPE) Global with a resolution of $1 \times 1^\circ$. This provides basis to help identify chemicals for which spatial differentiation will be important in LCAs, including whether differentiation will have added benefits over the use of global generic default values, such as those provided by the USEtox model.

Methodology A methodology was developed to explore spatial distribution and spatial variability of the fate of organic chemicals. Firstly, guidelines were developed to assign a hypothetical spatial distribution to chemicals which were clustered on the basis of their physical–chemical properties and persistence. Secondly, a test set of 34 representative organic chemicals was used to run MAPPE

Global and USEtox model. The results of MAPPE Global were used to highlight spatial variability of removal rate from air amongst different chemicals and their related patterns of variability. A comparison between USEtox and MAPPE Global removal rates from air was performed for each chemical in order to highlight whether spatial differentiation is relevant for the assessment or not.

Results and discussion Hypothetical spatial distribution of chemical fate was assigned to each combination of physical–chemical properties and persistence. Besides, spatial variability of removal rates from air was assessed running MAPPE model for the test set of 34 chemicals. The variability of results spans from less than one to over four orders of magnitude, showing differences in variability for each cluster of chemicals. Furthermore, different patterns of spatial variability are associated to each cluster of chemical as the spatial pattern is driven by a specific component of the overall removal rate. The comparison between MAPPE and USEtox removal rates from air shows that for 14 out of 34 chemicals within the test set, USEtox values are close to the median of the results of MAPPE. For 11 out of 34, USEtox underestimates the removal rate from air and the results are close to the fifth percentile of MAPPE ones. This is mainly related to how wet/dry deposition and gas exchange are accounted in the two models.

Conclusions and outlook This work has made further progress towards understanding and implementing how to develop a tailored-made guidance for assessing spatial differentiation in LCA. Results on spatial distribution and spatial variability of chemical are presented as a basis for defining patterns of variability and supporting further development of spatial scenarios and archetypes to be used for life cycle impact assessment. This provides insights into whether using generic global default factors is likely to result in high uncertainty depending on the type of

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chemical, as well as whether pattern-specific factors would reduce the uncertainty. Uncertainties related to spatial differentiation are presented and discussed.

Keywords Spatial differentiation · Spatial variability · Chemicals fate · Life cycle impact assessment of chemicals · Removal rates · USEtox · MAPPE model

1 Introduction

There is continual debate whether the exclusion of spatial information in applications such as life cycle assessment (LCA) may lead to misleading results, influencing the decision on products environmental performance (Finnveden et al. 2009).

Traditionally, LCA has been applied in a site-independent manner as emissions and resource consumption data are often not spatially and temporarily resolved. Many adopted impact assessment models provided generic results, as often is the case in screening chemical risk assessments performed, e.g., for policy support. Reasons can include political motives to, e.g., not distinguish between chemical risks in such assessments due to where an emission occurs. Equally, providing more spatial resolution can complicate assessments and may not reduce the uncertainty of the results.

In recent years, several research activities have been focused on identifying whether or not spatially detailed assessment is fundamental for decision support (e.g., Hauschild and Potting 2005; Pennington et al. 2005). In the context of life cycle impact assessment (LCIA), site-dependent characterization factors have been calculated for different impact categories, including for acidification and eutrophication (Seppälä et al. 2006; Gallego et al. 2010), photochemical ozone formation (van Zelm et al. 2008), ecotoxicity, and human toxicity (Wegener Sleeswijk and Heijungs 2010).

Toxicity-related impacts are argued to present high variability among different models (Huijbregts et al. 2003; Geisler et al. 2004), and results are sometimes expected to be highly sensitive to spatial differentiation—depending on emission patterns, chemical properties, location, and various other parameters.

In particular, for toxicity-related site-dependent assessment, there is an increasing demand for a balance between resolution required by models and complexity that can be handled given the quality of available data, the computational resources, as well as issues related to the availability of spatially/temporally resolved emissions data. No model can be a true representation of the real system, and optimal model performance can be only achieved by balancing the model's level of detail against

the demand for input parameters that are always uncertain (MacLeod et al. 2010).

Hence, it is necessary to further explore the uncertainties related to results derived from the straightforward multimedia models without spatial resolution that are often used in applications such as chemical risk and LCAs (where the variation in environmental characteristics are usually ignored and the analysis is limited to modeling typical or average environmental conditions) in comparison with spatially resolved models at various resolutions.

Besides, Wania and Mackay (1999) highlighted that non-spatially resolved multimedia models with low spatial and temporal resolution are appropriate for describing the behavior of persistent contaminants in the environment. The behavior of chemicals can be predicted directly from the physical–chemical properties, if this is the main purpose of the application. In other cases, detailed models can be necessary to introduce spatial differentiation and for more detailed, quantitative risk estimates. Several spatially resolved multimedia mass-balance models, at various resolution, were developed for chemical assessment and adopted as decision-support tools, such as Bert world (Toose et al. 2004), Impact 2002 (Pennington et al. 2005), Globox (Wegener Sleeswijk and Heijungs 2010).

Furthermore, both in chemical risk assessment and in LCA, the number of chemicals under assessment can be huge. Many chemicals do not present characteristic of persistent or long-range transport (LRT) pollutant but imply impact at local scale (e.g., the emission in urban air of a chemical with a very low half-life in air is foreseen to exert local effect).

To understand whether substance properties or environmental parameters are the key factors, several studies have explored (Hertwich and McKone 2001; Pennington et al. 2005; Hollander et al. 2009; Pistocchi et al. 2010) the relative influence of substance properties and environmental characteristic on the results of spatially explicit fate models. Substance properties such as partitioning between environmental phases (that define the chemical space of a chemical) and susceptibility to degradation are two major factors determining the fate and bioaccumulation of organic chemicals in the environment (Brown and Wania 2009; Wania 2006).

The study of Hollander et al. (2009), amongst others, showed that fate of chemicals in the environment depends mainly on these substance-specific partition coefficient and degradation rates. Nevertheless, the relative influence of environmental characteristics increases if models are run at a more detailed spatial scale. This was confirmed by, e.g., a case study on Canada, performed by Manneh et al. (2010) at three resolution scales, in which variability of the results decrease significantly at higher resolution.

To ensure robustness in discussing the uncertainties and the variability related to the use of a global default factors for risk/emission in applications such as LCA, instead of using spatially defined ones, a detailed assessment has to be carried out considering uncertainties and variability along the cause effect chain: fate, exposure, and effect. In this study, we decided to focus on the beginning of the environmental cause–effect chain (removal rates) in order to assess the variability associated with these factors.

The aim of this study is, firstly, to provide insight guidance into the drivers of spatial differentiation and, secondly, to assess spatial variability of atmospheric chemical removal rates using a global, spatially resolved multimedia model. The guidance on spatial differentiation and distribution is based on physical and chemical properties, while spatial variability assessment relies on the results of a complex and highly resolved global model Multimedia Assessment of Pollutant Pathways in the Environment (MAPPE) Global model (Pistocchi et al. 2011b). This allows identifying the pattern and extent of spatial differentiation and supports insights into whether spatial details are necessary in the context of chemical impact assessment.

A comparison between MAPPE Global and USEtox (Rosenbaum et al. 2008) box model parameters was performed at the level of air removal rates in order to discuss the uncertainties related to the use of generic impact assessment factors and to highlight the potential relevance of higher level of spatial detail in order to develop, in further steps, specific emission scenarios. The model were run for a test set of 34 chemical covering various portions of chemical space in order to assess the spatial variability associated with different physical–chemical properties.

2 Methodology

A complete assessment on spatial differentiation requires at least two levels of analysis:

- Assessment of spatial distribution (the range of potential environmental geographical distribution) in order to understand at which scale a chemical is typically distributed (local, regional, global, etc.) and
- assessment of spatial variability (the variability of the distribution and fate of a chemical among various scenarios, continents, countries).

The methodology to explore spatial distribution and spatial variability related to chemical fate in the environment was organized as follows:

1. Spatial distribution. We propose a framework to assess the hypothetical spatial distribution and optimal geographical resolution for the fate assessment of chem-

icals on the basis of their physical–chemical properties. Organic chemicals were clustered dividing chemical space according to likely similar environmental behavior. A range of likely geographical distribution was assigned to each chemical group.

2. Spatial variability. A representative test set of 34 chemicals was identified from previous research that covers likely chemical fate behavior. For each chemical of the test set, the spatially explicit multimedia model MAPPE was run to assess the variability of the results and to identify specific geographical patterns of variability. The analysis of the spatial variability was performed exploring variability in chemical removal rates from air.
3. Comparison of the results provided by MAPPE with the global default values provided by USEtox in order to assess the related uncertainties.

2.1 Spatial distribution of chemicals based on LRTP metrics

2.1.1 Clusters of organic chemicals

Persistence (P), long-range transport potential (LRTP), bioaccumulation (B), and toxicity (T) are characteristics directly related to a chemical's environmental risk (Muir and Howard 2006).

Since these characteristics are related to physical–chemical properties, organic chemicals were clustered on the basis of their physical–chemical properties in order to define a general framework for identifying groups of chemicals with likely similar fate behavior in the environment. This built on the previous work of the Omnitox project (Molander et al. 2004).

The framework was based on chemicals' equilibrium partition coefficients between octanol and water (K_{ow}), air and water (K_{aw}), and octanol and air (K_{oa}) and on chemical's persistence.

Firstly, the chemical space was divided in 16 subsections (1a, 2a, etc.) adapting the scheme proposed by Gouin et al. (2000), revised by Pennington et al. (2005) for non-dissociating and non-amphiphilic chemicals. Figure 1 presents the 16 subsections of the chemical space. The subsections are based on K_{ow} and K_{aw} partitioning coefficients according to similar environmental partitioning behavior. The 45° diagonals represent constant values of K_{oa} under the assumption of $\text{Log}K_{oa} = \text{Log}K_{ow} - \text{Log}K_{aw}$.

The range of physical–chemical properties of each subsection is defined in Table 1. The clusters are organized also in order to distinguish: fliers, multiple hoppers, swimmers, and single-hopper chemicals (Wania 2006). These definitions refer to the different behaviors of chemicals, based on their

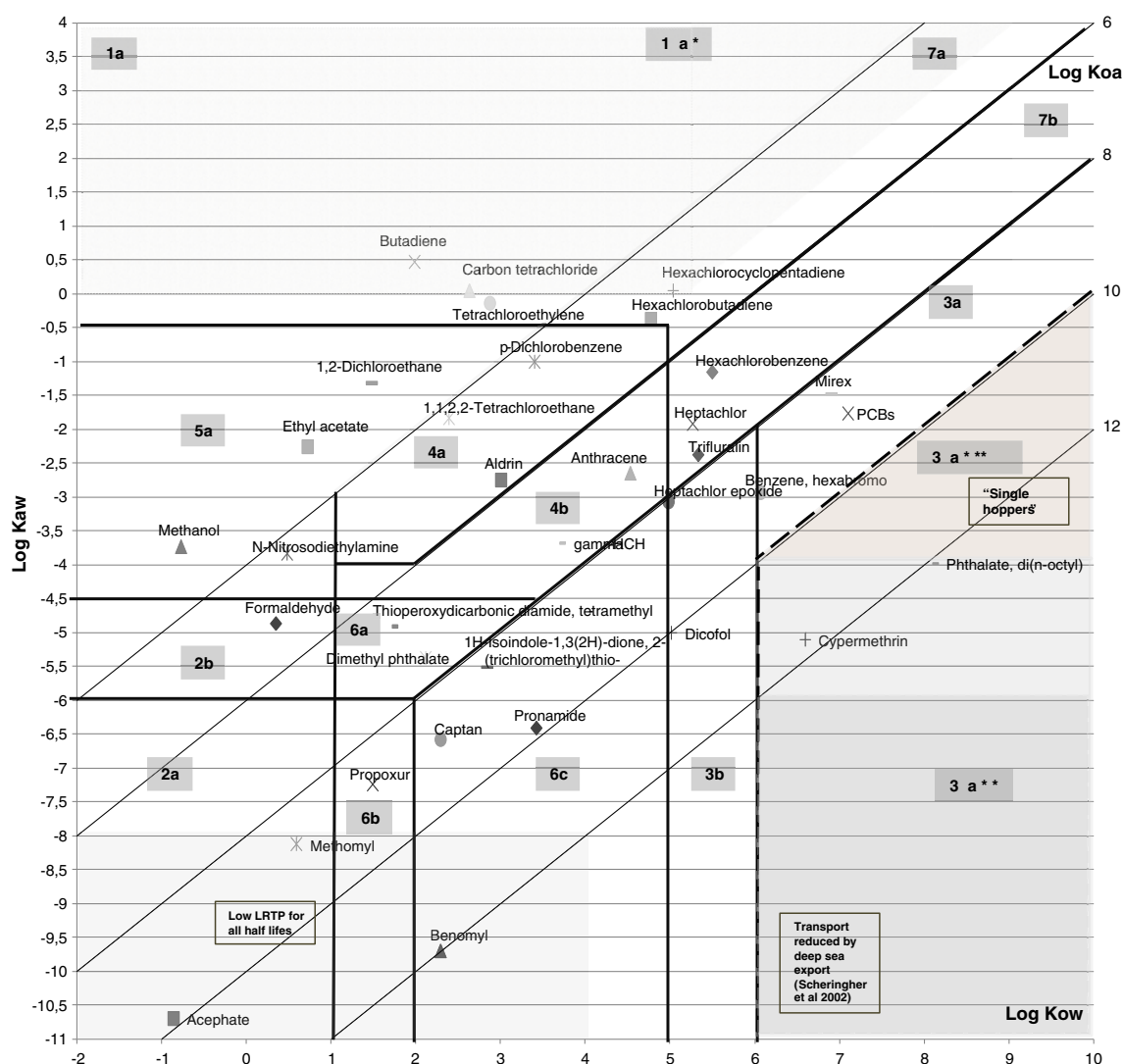


Fig. 1 Subsections of the chemical space (1a, 2a ...) with similar environmental behavior and location of the 34 representative chemicals in the test set

own properties: “fliers” are transported by air, “swimmers” present a low Henry's constant and are transported by water, “multiple hoppers” are semi-volatile chemicals in dynamic exchange between atmosphere and ocean, “single hoppers” generally present high Koa, and when they are deposited to soil, there is no revolatilisation.

2.1.2 Test set of chemicals

Within the chemical space, a so-called test set of 34 organic chemicals was adopted. The test set takes into account chemicals having a large diversity of physical–chemical properties in order to be representative, as far as possible, of their potential differences in the environmental behavior. Furthermore, these substances with these representative properties had already been used to assess multimedia fate of chemicals by Pennington et al. (2005) and for model

cross comparison in USEtox (Rosenbaum et al. 2008). The representative test set of chemicals and the associated physical–chemical data used in running the MAPPE model are listed in S1 of the supporting material. The position of each chemical within the chemical space is also plotted in Fig. 1.

2.1.3 Spatial distribution of chemicals based on physical–chemical properties

In defining guidance for spatial distribution, we considered how different chemical properties could be used to identify when a local, regional, or global assessment of chemical fate is needed. The guidance was developed by defining the hypothetical spatial distribution of a chemical on the basis of its physical–chemical properties, such as Kow, Koa, Kaw, and persistence.

Table 1 Guidance on spatial distribution of the chemicals based on LRT metrics (physical–chemical properties and persistence) for emissions in air

Subsections	Log K _{ow}	Log K _{aw}	Log K _{oa}	<1 day	1 day>>> 1 week	1 week>>< 1 months	>1 month	Main fate compartment
1a		>−0.5	<4	L	R/C	Co/G	Co/G	Air
1a ^a		>0	<6.5	R/C	G	Co/G	Co/G	Air (fliers)
2a	<1	<−6		L	R/C	Co/G	Co/G	Water
2b	<1	−4.5<×<−6		L	R/C	Co/G	Co/G	Water
3a	>6		>8	L	L	R/C	Co/G	Solid
3a ^b	>6	<−6		L	L	R/C	R/C	Solid
3a ^c			>10	L	L	R/C	R/C	Solid
3b	5<×<6		>8	L	L	Co/G	Co/G	Solid
4a	1<×<5	−4.5<×<−0.5	4<×<6	L	R/C	Co/G	Co/G	Multimedia
4b	1<×<5	−4.5<×<−0.5	6<×<8	L	R/C	Co/G	Co/G	Multimedia
5a		−4.5<×<−0.5	<4	L	R/C	Co/G	Co/G	Air–water
6a	1<×<4	−4.5<×<−6	6<×<8	L	L	Co/G	Co/G	Water–solid
6b	1<×<2	<−6		L	L	R/C	Co/G	Water–solid
6c	2<×<5	<−4.5	>8	L	L	R/C	Co/G	Water–solid
7a		>−0.5	4<×<6	L	R/C	Co/G	Co/G	Air–solid
7b	>5		6<×<8	L	R/C	Co/G	Co/G	Air–solid

L local scale (up to 10¹ Km), R/C regional/country scale (up to 10³ Km), Co/G continental/global scale (10⁴–10⁵ Km)

^a So volatile that they don't deposit to the Earth's surface, even under the condition of the Arctic Environment (Wania 2006)

^b Transport reduced by deep sea export (Scheringer et al. 2002)

^c Single hoppers, tending to be associated with particles in the atmosphere, usually deposited irreversibly to the Earth's surface (Wania 2006)

The guidance on spatial distribution is based on a flow chart (see Table 1) in which each cell represents a combination of:

- One of the 16 subsections of the chemical space, derived from the clustering made on the basis of specific chemical behavior and LRTP.
- One of the four classes of persistence (below 1 day, from 1 day up to 1 week, from 1 week up to 1 month, and more than 1 month). The classes were set taking into account that 2 days of half-life in air is considered a screening criteria for differentiating LRT chemicals from others (UNEP 2001). This might apply to substances emitted in parts of temperate Europe, North America, or Asia, for example, and then traveling with some efficiency to reach the Arctic (Scheringer et al. 2009).

For each combination of chemical properties and persistence, the hypothetical spatial distributions was assigned on the basis of the results of the OECD “Tool” (Wegmann et al. 2009) and of literature review on patterns of spatial distribution of LRT chemicals.

2.2 “The Tool” by OECD and spatial distribution of LRT chemicals

“The Tool” is the overall environmental persistence (Pov) and LRTP screening tool recently released by the Organization for

Economic Cooperation and Development (OECD 2010; Wegmann et al. 2009). This is a harmonized approach for assessment of overall persistence (Pov) and LRTP on the basis of physical–chemical properties of chemicals. The Tool represents the consensus of current multimedia model assessment methods to calculate the overall environmental persistence (Pov) and characteristic travel distance (CTD) as described by Beyer et al. (2000) and transfer efficiency (TE) as described by Macleod and Mackay (2004), as metrics for LRTP (Wegmann et al. 2009).

The Tools came from the study of Fenner et al. (2005) in which nine different multimedia models were assessed. Significant differences among the nine models assessed by Fenner et al. (2005) have been shown to be restricted to a certain region of the chemical space. This suggests that for the other areas of the chemical space, the models predict similar behavior of chemicals in term of Pov and LRTP.

Hence, the combination of LRTP (based on Kow, Kaw, and Koa) and persistence (Gouin 2010) supports the identification of the hypothetical spatial distribution, for assessing the fate of chemical as presented in Table 1 in accordance with The Tool results.

A further cross-checking with studies on LRTP patterns was performed to support assigning the spatial distribution to each combination in Table 1.

For example, the Arctic Contamination Potential (Wania 2006) indicates that some LRTP chemicals are subject to a

specific pattern of distribution in the environment, and for those substances, the preferred scale of assessment is the global one. This is confirmed also by monitoring campaigns, such as the comprehensive study of patterns of distribution (Macdonal et al. 2000) developed under the Canadian Northern Contaminants Program which has enhanced the understanding of the pathways by which contaminants reach Arctic and move through terrestrial and marine ecosystems. Other studies (Toose et al. 2004) identified significant source-to-sink pathways and processes in the LRT of chemical to Arctic regions. For substances that degrade faster in water than in soil, but are quite persistent in the atmosphere, or that are soluble and highly persistent in water, highest Arctic contamination is expected to occur if the substances have intermediate volatility and high hydrophobicity.

2.2.1 How to use the guidance on spatial distribution

Ideally, an LCA practitioner has to identify the chemicals representing the major contributors to the toxicity-related impact, checking, then, where the chemicals are located in the chemical space to easily identify the potential spatial distribution of the chemicals under assessment according to Table 1.

Considering, e.g., carbon tetrachloride (CCl_4), for its physical–chemical properties, it is in the subsection 1a. As CCl_4 half-life in air in the literature spans from 3 to 5 months, it can be considered as a chemical with a high potential of being globally distributed. This is confirmed by the result of the “The Tool”, in which it presents both high CTD and high TE. Therefore, the chemical should be considered as a global contaminant to be assessed at global scale. Indeed, the place of emission and the place of the potential related impact may be very distant.

On the other hand, highly hydrophobic chemicals (like 3a) with low-to-moderate persistence are expected to have a local/regional spatial distribution. This may affect the result of the impact assessment, especially for specific routes of exposures, such as implication for human intake fraction via inhalation.

For chemicals distributing from continental to global scale, it is expected that the place of emission and the place of impact may be distant and, therefore, global models at low resolution can be suitable for the impact assessment. On the other hand, for chemicals distributing locally or regionally, models at higher resolution are preferable, as the major contribution to impact is related to local condition. In the latter case, as shown also by Hollander et al. (2009), the role of environmental parameters became more relevant than the mere physical–chemical properties.

2.3 Spatial variability of removal rates for the test set of chemicals

Knowing the hypothetical spatial distribution, a second relevant step is to assess the spatial variability and whether or not to proceed with a site-specific assessment. As mentioned above, the choice is not only related to the hypothetical spatial distribution of a chemical, based on its physical–chemical properties, but also on specific environmental parameters that may influence the final result.

Referring to Table 1, we may argue that for highly hydrophobic chemicals with low persistence (although the scale of their spatial distribution is local), we may rely on global site-independent approach. Irrespective of specific location of emission, they will present low spatial variability of the fate. Indeed, fate of chemicals in the environment is much more affected by chemical properties than by environmental conditions when the chemical present very extreme partitioning properties. Wherever the emission takes place, we can assume that the behavior is similar.

This assumption can be applied also for chemicals with LRTP that are subject to specific spatial pattern (e.g., those that present a high arctic contamination potential): in this case, highly detailed information on the source of emission has a limited influence on the final fate calculations.

Therefore, the need for spatial differentiation was further explored combining the assessment based on physical–chemical properties with the assessment of specific environmental parameters leading to specific “patterns” of spatial distribution and variability.

The variability in the chemical behavior and the potential related patterns were identified with the spatially resolved MAPPE Global model. The analysis of the variability of removal rates from air (K_{air}) governing environmental fate of chemicals emitted in air was the starting point for the assessment.

K_{air} total is the sum of five removal rate processes: particle dry deposition (K_{part}), wet deposition (K_{wet}), gas absorption (K_{gas}), degradation (K_{deg}), and advection (K_{adv}).

$$K_{\text{air}} = K_{\text{part}} + K_{\text{wet}} + K_{\text{gas}} + K_{\text{deg}} + K_{\text{adv}} \quad (1)$$

At equal emission rates (1 U of emission), the air removal rates are expected to be different for different groups of chemicals and for different environmental conditions. Under this assumption, MAPPE Global model was run in order to assess the spatial variability in the removal rates for the test set of chemicals.

2.4 The global multimedia assessment of pollutants pathways in the environment—MAPPE global model

MAPPE Global is a GIS-based model that builds on the concept of the previous MAPPE Europe version (Pistocchi 2008; Pistocchi et al. 2010). MAPPE Global is a spatially resolved steady-state multimedia model (i.e., the rate coefficients are not temporally resolved in current version). The detailed model description, background parameters and input data are reported in Pistocchi et al. (2011b) (see also S2).

Currently, MAPPE computes only the removal rates of a substance with given physicochemical properties. It is composed of atmospheric boundary layer, soil, inland, and seawater, for the whole world, with a resolution of $1 \times 1^\circ$ (except for some parameters, which are defined at finer resolution). Advection at the global scale between cells is not yet modeled. Hence, the influence of distributing an emission over a region, which would reduce the maximum potential variability for some types of chemical, is not modeled at the global scale.

The MAPPE Global computes, for each grid cell, mass fluxes of chemical that are available for transport outside of the cell and their global variability. MAPPE Global is developed specifically to answer questions concerning the environmental fate of contaminants taking into account the variability of environmental processes at the global scale and the variability of fate in response to spatial variability of emissions and chemical fate processes, such as:

- How will a chemical spread across different media in different climatic and landscape settings?
- How important is the variability of environmental processes in determining the fate of chemicals across the globe?
- How much of a chemical emitted to air will result in a load to soil or waters?

With respect to spatial differentiation, MAPPE Global allows: adopting several scales of assessment by differentiating on the basis of grid cells (100×100 km), political boundaries (countries), or geographical borders (river basins, continents, global); and identifying specific patterns in the environmental behavior of chemicals.

2.5 Comparison MAPPE versus USEtox

Straightforward non-spatial multimedia models are widely used in LCIA for modeling chemical fate and human exposure. USEtox reflects a latest consensus amongst LCA model developers for the calculation human and ecotoxicity characterization factors amongst associated multimedia models. The aim of the comparison was to understand the

maximum level of uncertainty associated with the use of such a global default value provided by USEtox, by applying a multimedia model with a spatial resolution of $1 \times 1^\circ$, in this case, MAPPE. To highlight the variability of factors at the beginning of the environmental cause–effect chain, the comparison was made at the level of the removal rates coefficients.

USEtox has been set up to model a global default continent, and it has a nested multimedia model in which it is possible to consider global, continental (with six environmental compartments), and urban scale differentiation.

In Fig. S1, all the organic chemicals presented in the USEtox database are plotted. Most of the chemicals are within the chemical space of Fig. 1. Few other substances, with extreme partitioning properties are outside. These will have extreme behavior in partitioning either in air, in soil, or in water. In Fig. S2, the position of chemicals within the chemical space defined in this paper is shown, and for them, the guidance on spatial distribution can be applied. Furthermore, it is relevant to note that over a half of the chemicals in the USEtox database (Fig. S3) have half-lives in air less than 1 day. Following the indication in Table 1, for many of those chemicals, a local spatial distribution is foreseen to be relevant.

3 Results and discussion

The MAPPE Global model was run in order to highlight the maximum spatial variability of the removal rate coefficients considering emissions in air of 1 U of chemical in each cell of $1 \times 1^\circ$ in which the globe is divided, in order to:

- assess the global variability of removal rates from air for the test set of 34 chemicals, identifying associated patterns of spatial variability for chemical's clusters
- and compare the results of MAPPE and USEtox.

3.1 Global variability of removal rates from air and associated patterns

In a first screening calculation, we ran MAPPE for the 34 chemicals considering all the five removal processes from air: particle dry deposition (K_{part}) and wet deposition (K_{wet}), gas exchange (K_{gas}), degradation (K_{deg}), and advection (K_{adv}). The results (see Fig. S4) evidenced that 30 out of 34 chemicals have variability in global values below one order of magnitude if we consider the total K_{air} , including the advection. In the case of Aldrin, the variability is even less than one order. Propoxur and Benomyl are over one order of magnitude but below two. Two chemicals, representative of the 2a class, present a

high variability: Methomyl almost three orders of magnitude while Acephate over four orders of magnitude.

Secondly, as we want to focus the assessment on the variability at local scale, the analysis was performed without advection and considering only the other four removal processes: (Kpart, Kwet, Kgas, and Kdeg). The results of the variability (median, 5% and 95% quantiles) are presented in Fig. 2, clustered by order of magnitude of variability in Table 2. Background data are reported in Table S2.

In general, the variability of the chemicals spans from less than one up to more than four orders of magnitude. These results support the need of assessing separately the potential spatial distribution of a chemical (local, regional, at country level, etc.) and its spatial variability.

The comparison of the variability of results with and without advection (Fig. S4 and Fig. 2) implies that for persistent chemicals, the advection will be more important compared to the other removal processes. It is worth to highlight that the variability of removal rates as a function of location will thus be reduced, due to an averaging over space associated with dispersion.

Besides, chemicals in the same classes (e.g., 3a) do not present the same variability of the removal rates. Chemicals such as di(n-octyl)phthalate and Cypermethrin show a very low variability (less than one order of magnitude), whereas hexabromobenzene shows a variability of more than four orders of magnitude, PCBs and Mirex over two orders.

For almost all the chemical in the test set, the extended ranges of variability are observed in the area below median values, while for all chemicals, the variability over the medians is up to one order of magnitude.

Hence, for chemicals that present high variability of Kair, it is necessary to explore the sources of this variability in order to identify main related drivers and geographical patterns.

Aiming at identifying reasons for variability and at specifying whether the variability follows similar spatial patterns for different chemicals, maps of distribution of values at global scale were calculated. Actually, maps could be used not only to visualize but also to analyze the spatial nature of pollutants (Lahr and Kooistra 2010). Analyzing the spatial patterns in the maps of the chemicals (all available in the [Electronic supplementary material](#)), the variability of the results in Fig. 2 could be explained as follows.

For chemicals in the group 1a, the dominant compartment is air. The variability could be driven by gas exchange in the atmosphere that basically depends on the variability of land cover. See for example, for Butadiene, the map removal rate from air without advection (Fig. S5). Comparing the spatial pattern of the Kair with the pattern of Kgas, it is confirmed that there is a dependence of the final result on the variability of the gas exchange, and the differences in the global distribution of land cover influence the variability of the results (Fig. S6).

The environmental partitioning of 2a chemicals is mainly related to water. The high variability in the Kair values could be explained by the difference in the precipitation among countries. Comparing the total removal rate of a highly hydrophilic chemical, such as the acephate (Fig. S7), with the pattern of the map of the wet deposition removal rate (Fig. S8) and the pattern of the annual average precipitation map (Fig. S9), it is clear that the foremost

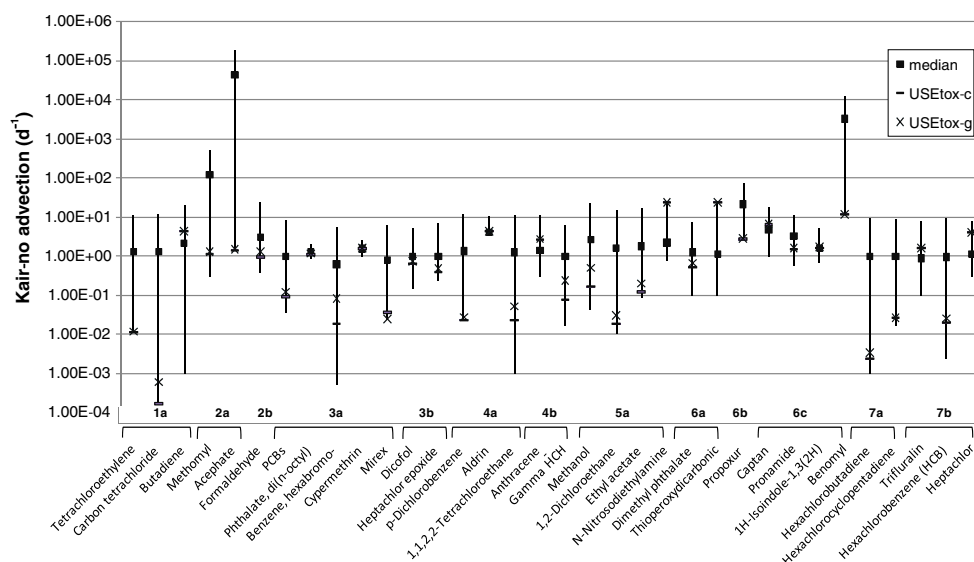


Fig. 2 Variability of removal rate from air (Kair total in liter per day) for the test set of 34 representative chemicals (no advection case). Results plotted: MAPPE median (*black squares*), 5th and 95th

percentile values at $1 \times 1^\circ$ of resolution; USEtox (*lines*) continental and (*multiplication signs*) global default values

Table 2 Variability of the removal rates from air for the 34 chemicals in the test set

<1 order of magnitude		1<×<2	2<×<3	3<×<4	×>4
1a			Tetrachloroethylene 1a	Carbon tetrachloride 1a	Butadiene 1a
2a			Methomyl 2a		Acephate 2a
2b		Formaldehyde 2b			
3a	Phthalate, di(n-octyl) 3a Cypermethrin 3a	Mirex 3a	PCBs 3a		Benzene, hexabromo- 3a
3b		Dicofol 3b Heptachlor epoxide 3b			
4a	Aldrin 4a		p-Dichlorobenzene 4a		1,1,2,2-Tetrachloroethane 4a
4b		Anthracene 4b Dimethyl phthalate 4b	Gamma-HCH 4b		
5a		N-Nitrosodiethylamine 5a	Methanol 5a Ethyl acetate 5a	1,2-Dichloroethane 5a	
6a		Thioperoxydicarbonic diamide, tetramethyl- 6a			
6b		Propoxur 6b			
6c	1H-Isoindole-1,3 (2H)-dione, 2- (trichlor) 6c	Pronamide 6c Captan 6c Benomyl 6c			
7a			Hexachlorocyclopentadiene 7a	Hexachlorobutadiene 7a	
7b		Trifluralin 7b Heptachlor 7b		Hexachlorobenzene (HCB) 7b	

Orders of magnitude of difference between 5th and 95th percentile are presented

removal rate process is the wet deposition. The same explanation may describe the spatial variability of Methomyl, also in the 2a group but less hydrophilic (Fig. S10).

In the case of hydrophobic chemicals with a low affinity for air, such as PCBs in the 3a group, the pattern of variability may be explained considering those chemicals emitted to air, with gas absorption (Figs. S11 and S12). However, the additional pattern map (Figs. S13–14) shows that a certain influence of K_{part} could be accounted for the total variability, as the highest values in the total removal rate are in the same areas where particle dry deposition is uppermost.

Furthermore, for explaining the different variability amongst chemicals within 3a (e.g., cypermethrin and hexabromobenzene), a combination of the role of degradation rate and the variability of the K_{gas} has to be taken into account. The variability of gas exchange drives (Figs. S15 and S17) the overall variability of the K_{air} when the degradation rate is low (as in the case of hexacromobenzene— $4.9 \cdot 10^{-4}$ 1/day) and the persistence is high (over 1,000 days of half-life in air). In the opposite case, where the degradation rate is higher (as cypermethrin—0.92 1/day or di(n-octyl) phthalate—0.89 1/day) and the persistence is low (0.75 and 0.78 days, respectively, of half-life in air) the overall variability is very low (Fig. S18). Then, the degradation, as an elimination process from atmosphere, reduces the range

of variability of total air removal rates, which potentially express a large variability due to the wide spatial fluctuations of gas exchange or wet/dry deposition. This means that it is not possible to assign spatial variability to a certain group of chemicals based only on the partitioning properties without accounting for the role of degradation.

For multimedia chemicals, like those in 4b, the pattern of variability is related to the interplay of different removal rates (see Figs. S19–S23) even if substantial contribution is still related to gas exchange since the K_{gas} is the prevailing removal rate compared to the others. In Fig. S24, an example for lindane is presented, showing variability of removal rates across countries where K_{gas} and K_{wet} present variability over three orders of magnitude, while K_{deg} and K_{part} around one order.

3.2 Comparison of removal rates from air: MAPPE versus USEtox

The comparison MAPPE versus USEtox was performed in order to assess the total air removal rates (K_{air}) calculated by running a multimedia model with default environmental parameters and no spatial resolution against MAPPE with a spatial resolution of $1 \times 1^\circ$.

Since we are exploring the variability at the very beginning of the environmental cause–effect chain, the

comparison covered only contrasting removal rate coefficients from air to assess the uncertainties related to a site-generic approach, such as the one proposed by USEtox.

The USEtox results were calculated keeping as they are the default environmental parameters provided by the model. The removal rates for continental and global scale were calculated specifying the values of removal to stratosphere, degradation, wet and dry deposition, and gas adsorption.

In Fig. 2 and Table S2 and Fig. S25, the results of USEtox also are reported.

The model comparison shows that for 14 (such as formaldehyde 2b, cypermethrin 3a, aldrin 4a, and N-Nitrosodiethylamine 5a) out of 34 representative substances the median of the total air removal rates calculated with MAPPE is within one order of magnitude of difference with USEtox. For almost all the tested substances, the USEtox values are below the median values calculated by MAPPE. The only exceptions are: butadiene, anthracene, N-Nitrosodiethylamine, tetramethyl-thioperoxydicarbonic diamide (thiram), trifluralin, and heptachlor. In general, USEtox tends to underestimate MAPPE Global estimates for the removal rates between one and four orders of magnitude and the USEtox values are close to the fifth percentile of the MAPPE results for 7 out of 34 chemicals.

Moreover, for the groups of flyers (1a) or hydrophilic substances (2a, 7a), the underrating is higher and varies from two up to almost four orders (maximum deviation observed for acephate 2a)

It is worthy to highlight that in case of low variability of the MAPPE results worldwide (as for di(n-octyl)phthalate, cypermethrin, aldrin, and folpet), the USEtox value is very close to the median. At higher variability, the uncertainties (difference of global default value from the median of the spatially resolved one) associated to the global default values increase.

Assuming equal chemical properties, two main factors may lead to the discrepancies: different algorithms to calculate the removal rates; variability of environmental parameters in MAPPE compared to the environmental parameters in the default setting of USEtox.

Analyzing the results in Fig. 2 and in Fig. S25, the following conclusions can be drawn:

For chemical for which the removal rate is dominated by wet and dry deposition (as e.g., 2a), MAPPE results show a higher variability due to a broader range of average rain rate across the globe (fixed value in USEtox, 700 mm year⁻¹; values in MAPPE, 600–3,600 mm year⁻¹). Furthermore, MAPPE does not consider intermittent rain conditions, whereas USEtox accounts for that. This may explain the different estimation of *K*_{wet}.

For chemical for which the removal rate from air is dominated by gas exchange (as e.g., 1a), MAPPE results

present a variability associated with different land coverage. As explained in the [Electronic supplementary material](#), MAPPE accounts for different gas exchange for various land coverage, assuming broad differences in gas absorption velocity and in related coefficient. Specifically, MAPPE assigns higher gas exchange coefficient to different forested areas compared to USEtox.

For chemical for which the degradation rate in air is much higher than the other removal rates (e.g., butadiene, N-Nitrosodiethylamine, tetramethyl-thioperoxydicarbonic diamide, heptachlor), USEtox tends to overestimate the MAPPE results (e.g., N-Nitrosodiethylamine and thiram).

Further research is needed to give a better insight on the reason behind the spatial variability and the associated discrepancies in the results. Once the full documentation of the algorithms behind USEtox will be available, a comprehensive sensitivity analysis of the parameters of the two models may help in identifying further differences and drivers of uncertainties. Anyway, this was beyond the scope of this study.

4 Conclusions

This study is based on a comparison of the result of a detailed spatially resolved model, computational intensive but useful to understand better specific patterns in spatial differentiation, against a simplified approach to the assessment of chemicals, provided by model such as USEtox, in order to identify key drivers of variability/uncertainties. The main results show the importance of assessing both spatial distribution and spatial variability to provide guidance on spatial differentiation for the specific purpose of LCA. Summarizing, the key findings are the following:

- Spatial distribution of chemicals could be identified through a guidance based on physical–chemical properties and persistence of chemicals, following the results of the OECD Tool (Wegmann et al. 2009) and literature review.
- Spatial variability in removal rate from air is different for various clusters of chemicals due to the interplay of physical–chemical properties and degradation rates. The variability increases especially for chemical with low air degradation rate. This means that it is not possible to assign spatial variability to a certain group of chemicals based only on the partitioning properties without accounting for the role of degradation.
- Spatial variability is associated to different spatial patterns, due to the influence of specific removal rate for each cluster of chemicals. In this paper, relevant patterns affecting variability of removal rates were identified, supporting the need of considering both

physical–chemical properties and environmental parameters in assessing chemical fate.

- The comparison of the USEtox model and the spatially resolved model MAPPE for the removal rate coefficient from air revealed discrepancies that span from one up to four orders of magnitude. The differences are mainly due to the removal rates related to wet/dry deposition and gas exchange. A comprehensive sensitivity analysis may give further insight in order to address uncertainties related to specific differences in the algorithms and in the default model setting of USEtox.

5 Outlook and recommendations

This work has made further progress towards understanding and implementing how to develop a tailored-made guidance for the specific purpose of assessing spatial differentiation in LCA. Nevertheless, some issues need to be addressed in further research activities. Nowadays, the real challenge for spatial differentiation is a transition from theoretical framework towards feasible and reliable approaches, tackling some relevant issues.

5.1 Role of advection

Although this issue was beyond the scope of this study, the advection represents the major process contributing to the transport of LRT chemicals among countries and spatial variability analysis have to be conducted at various scale of resolution.

5.2 Not only LRT chemicals

So far, research efforts were mainly dedicated in identifying LRT chemical that can act as global chemical. Nevertheless, an effort is required also for identifying suitable scale for the impact assessment of others chemicals. Although these substances are not POP or LRTP, they may locally affect human health and ecosystems due to their high local concentration or to their high toxicity.

5.3 Sensitivity analysis

Sensitivity analysis (study of impact of input parameters on the value of outputs) has to be carried out to identify the key parameters affecting variability and patterns. This is particularly useful in supporting the definition of relevant scenarios and archetypes as well as understanding which data are the key input data for each chemical cluster and the key removal mechanisms. This is crucial also to better understand the key parameters affecting the discrepancies found between USEtox and MAPPE results. The environ-

mental parameters to be considered may be classified into geometric parameters (e.g., atmospheric mixing height), process parameters (e.g., dry deposition velocity), and compartment property data.

5.4 Framework for assessing uncertainties and variability

A common framework for assessing uncertainties and variability to be adopted in LCA is required and has to be conducted step by step along the environmental cause–effect chain. According to Meyer et al. (2005), the study of uncertainty has to be distinguished in the study of the uncertainty of the input parameters on the uncertainty of output parameters, highlighting variability (spatial and temporal variation in the environmental parameters), and true uncertainty (deficiencies in knowledge). Therefore, further comparison and assessment have to be conducted not only on the final results (e.g., variability in characterization factors) but also in the intermediate steps, considering parameter uncertainties, model uncertainties, and temporal variability.

Parameter uncertainty: The main source of uncertainties is related to physicochemical properties of chemicals in the environment (degradation half-lives and partition coefficients), and they need to be characterized and taken into account from the very beginning of any chemicals assessment (Boethling et al. 2009; Rosenbaum et al. 2008). Indeed, MAPPE requires the input of at least two partition coefficients (Kow, Kaw, or Koa) and three or four degradation rate constants or half-lives for air, water, soil and, sometimes, sediment.

Model uncertainty: The set up of the model involves uncertainties because the model structure and the selection of environmental processes always give an incomplete representation of reality based on knowledge and objectives of the model developer (Scheringer et al. 2009). MAPPE is a steady-state model with first-order removal process. As other similar model, this implies model's uncertainty as, e.g., in the model, the feedback effect is not considered as its importance is limited for most organic chemical (Margni et al. 2004). Furthermore, for the specific purpose of spatial models evaluation, Monte Carlo simulations are among the methods most commonly applied for the analysis of parameter's uncertainty. We did not use it for assessing variability/uncertainties in this study since Montecarlo simulation of spatial parameters in box models can significantly overestimate the realistic effect of spatial variation (Hollander et al. 2009). A promising method to assess uncertainty and uncertainty propagation was presented by Hong et al. (2010). Besides, for a comprehensive uncertainty assessment, there is the need of comparing model results at various resolutions, under different background parameter assumption, and also with measured

real data. At the actual stage of site-specific model's development, the model validation is often limited to local situation and rarely validated at wider scale (continental or even global).

Temporal variability: All the calculations are based on average annual values of input parameters. Therefore, temporal/seasonal variation is not taken into account but may affect the final result of the removal rates (e.g., when discrete events such as precipitation are temporally averaged)

5.5 Patterns of spatial variability

Recently, a discussion on the state of art and perspectives in spatially explicit multimedia fate models (Pistocchi et al. 2010, 2011a) has highlighted that the key question to be addressed is not anymore “how to compute” (numerical methods, spatial temporal discretization, quantitative uncertainty, and sensitivity analysis) but “what to compute”. This suggests concentrating the effort in understanding spatial patterns of both emission and environmental key drivers.

5.6 Substance or space: not only a matter of resolution

We may conclude that whether site-dependent factors reduce uncertainty compared to using generic defaults depends on the physical–chemical properties of the chemical under assessment and the environmental scenario in which the emission occur. A further development of guidance on spatial differentiation has to be chemical-specific and scenario-dependent.

5.7 Use of map for communicating

The potential benefit for communicating LCIA results in the form of maps has to be further explored. Nevertheless, it is important to help LCA practitioners to easily identify situations for which spatial differentiation in the LCIA of chemicals should be considered relevant.

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